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APPLICATION OF CRYSTAL LATTICE DISINTEGRATION CRITERIA TO COMPUTE MINIMUM SHOCK INDUCED REACTIVE CONDITIONS IN SOLID EXPLOSIVES AND INERT MATERIALS

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Consequently, it is tentatively concluded that crystal lattice breakup, or self-sustained phonon fission as Fitzgerald calls it, is responsible for the initiation of detonation in shocked explosives and enhanced thermocouple output in shocked materials.

Several recommendations for future work are given.

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I. INTRODUCTION

While engaged in a study of solid explosive detonation via small projectile impact, Reference [1], a scheme was developed to theoretically compute the lowest one-dimensional shock pressure required to initiate reactions leading to detonation in a solid explosive.

A threshold particle velocity criteria derived by E. R. Fitzgerald [2] for the onset of crystal lattice disintegration has been shown to agree rather well with the lowest particle velocity, and hence, shock velocity and/or shock pressure required to initiate reactions leading to detonation in certain explosives. In addition, the relation has also been employed to compute the lattice breakup shock conditions for an inert nonexplosive material, polymethyl methacrylate (PMMA). This result agreed well with an experimentally observed shock pressure level; above which shocked thermocouple output increased rapidly with increased shock pressure.

Similar shocked thermocouple data were also available for one explosive, PBX-9404. The computed lattice breakup shock pressure for PBX-9404 agrees rather well with both the pressure level for increased thermocouple response, and the experimental shock pressure necessary to initiate reactions leading to detonation.

It is known that a porous explosive requires less shock pressure to initiate detonation than the same explosive which is less porous or more dense. It is shown analytically and numerically that the shock pressures (or particle velocity) necessary for crystal lattice breakup also decreases as the material density decreases. This is suggested as an explanation of the observed porosity sensitivity effect.

Although additional investigation is needed, it is tentatively concluded that the onset of crystal lattice disintegration is responsible for reactions leading to detonation of explosions via shock pressure input. Also, it is physically plausible that crystal lattice fracture is responsible for the enhanced thermocouple response above a certain pressure level in shocked materials.

II. FITZGERALD'S CRYSTAL LATTICE FRACTURE OR DISINTEGRATION PARTICLE VELOCITY CRITERIA

From particle dynamics considerations, Fitzgerald ([2], Chapter III) derived the following relation for the velocity of a particle (in a crystal lattice) necessary to produce lattice disintegration. He called this the phonon fission velocity, V_f , which is:

$$v_{f} = \frac{v_{1} + \sqrt{v_{1}^{2} + 4 + v_{1} + c_{s}}}{2}$$
 (1)

It is approximately equal to:

$$V_{f} = \sqrt{V_{1} \star C_{S}} \tag{2}$$

the velocities V_1 and C_s are defined as follows:

$$V_1 = \frac{h}{2 m d_1} \tag{3}$$

= limiting free particle velocity which can occur without permanent lattice deformation (plastic flow); or the limit propagation velocity for particle-momentum waves in a stationary lattice.

$$C_8 = \sqrt{\frac{2 + c_t^2 + c_1^2}{6}}$$
 (4)

= A mean sound velocity defined such that the dissociation energy of an atom of mass, m, is m ${\rm C_s}^2$

The quantities appearing on the right-hand side of Equations (Eqs.) (3) and (4) are defined as follows:

h = Planck's constant

=
$$6.626196 \times 10^{-27} \frac{(gram) (cm^2)}{sec}$$

 d_1 = Closest distance between the atoms in a crystal lattice, or the atomic spacing in a slip direction. Units are angstrom units, A° (A° = 10^{-8} cm)

m = Mass of one atom, grams.

 C_t = Elastic transverse or shear wave velocity, cm/μ - sec

 C_1 = Elastic longitudinal wave velocity, cm/μ - sec

With respect to V_f , Fitzgerald points out that self-sustained fission is possible if fragments of the broken lattice strike other lattice sections and the process is repeated. Then he says: "The explosive nature of certain fractures may arise from this source," ([2], p. 81).

III. MINIMUM CRYSTAL LATTICE FRACTURE SHOCK VELOCITY AND SHOCK PRESSURE

Consequently, it seemed likely that lattice breakup phenomena could also initiate reactions leading to detonation in explosives. If so, then $V_{\rm f}$ would be the minimum particle velocity (due to impact or shock) required to cause detonation for one-dimensional large sample conditions. The corresponding shock velocity, $U_{\rm sf}$, and shock pressure, $P_{\rm sf}$, are:

$$U_{sf} = Co + S * V_f$$
 (5)

$$P_{sf} = \rho_0 U_{sf} V_f \tag{6}$$

With respect to Eq. 5, experimental results reveal that the shock velocity is a linear function of the particle velocity for many materials. Co and S (a constant) have been determined for many metals, plastics, and explosives ([3] through [7]). Co is a constant also, and is equal to the bulk sound velocity for most materials. The shock velocity may be a nonlinear function of the particle velocity for certain substances. In that case, $U_{\rm S}$ can be found from tables or graphs of $U_{\rm S}$ as a function of Up. Table 1 contains Co and S information for the shocked explosives and materials considered in this report. The sources of this information are also listed.

Equation (6) is the well known expression for shock pressure. P_{sf} is the product of the material density (ρ_0) , shock velocity (U_{sf}) , and the particle velocity (V_f) .

Numerical values of the three quantities, $V_{\rm f}$, $U_{\rm 8f}$, and $P_{\rm 8f}$ may, thus, be computed and compared with experimental data for any phenonmena which might be associated with lattice disintegration.

The particle fracture velocity V_f , is a function of two velocities, V_1 , and C_S , via Eqs. (1) or (2). The computation of V_1 requires the knowledge of two quantities, m, and d_1 . For the compounds and mixtures considered herein, m is m_{av} , the average weight of a single atom in the material. It is a constant for a given material and can be computed from the chemical formula or composition information. The distance d_1 will be a function of the density or specific weight (ρ_0) and m_{av} . It is computed as follows:

$$N_{V} = \frac{\rho_{O}}{m_{AV}} = \frac{(Grams)}{\frac{Cm^{3}}{(Grams)}} = \frac{Atoms}{cm^{3}}$$
 (7)

Considering that each atom, on the average, occupies a small cube whose side is d_1 , then

$$d_1^3 = \frac{1}{N_V} = \frac{m_{aV}}{\rho_0} = cm^3$$
 (8)

$$d_1 = \left(\frac{m_{av}}{\rho_0}\right)^{1/3} = cm \tag{9}$$

Thus, from Eqs. (3) and (9):

$$V_1 = \frac{h (\rho_0)^{1/3}}{2 (m_{av})^{4/3}}$$
 (10)

Since h is a constant, and for a given material, \mathbf{m}_{aV} is a constant, then:

$$V_1 = K (\rho_0)^{1/3}$$
 (11)

Where:

$$K = \frac{h}{2 (m_{av})^{4/3}}$$
 (12)

From Eq. (11), V_1 will decrease as the density decreases, or as the material becomes more porous.

The elastic wave velocities, C_1 and C_t , will normally decrease as the consity decreases also. Thus, from Eq.(4), C_8 will also decrease as the material becomes less dense or more porous.

It follows, then, from Eqs. (1) and (2), that $V_{\rm f}$ will decrease as the density decreases or porosity increases.

The shock velocity, U_{8f} , will be affected by porosity also; not only by the V_f or particle velocity contribution (Eq. (5)), but the form of the relationship may change. In general, the shock velocity will decrease (for a given particle velocity) as the density decreases or porosity increases. Note the characteristics of Tetryl described in [20].

Finally, the lattice fracture shock pressure, P_{6f} , will decrease via the product $(\rho_0^* U_{8f}^* V_f)$ as the density decreases and porosity increases.

The variation of $V_f,\ U_{Sf},$ and P_{Sf} with material density (ρ_O) has an important implication which will be discussed in Section IV.

Refinements, with respect to the computation of V_1 , appear feasible. Particular atoms or combinations of atoms and their associated minimum slip distances, d_1 , could be given special attention.

IV. THEORETICAL AND EXPERIMENTAL REACTION THRESHOLD SHOCK CONDITIONS FOR EXPLOSIVE AND INERT MATERIALS

 $V_{\rm f},~U_{\rm sf}$, and $P_{\rm sf}$ were computed for six high explosives and one inert material for comparison with selected experimental results. The six explosives were: Comp-B3, Comp-B, TNT (pressed), PBX-9404, Tetryl, and H-6. The inert material was Plexiglas II, UVA, which is also called PMMA. The pertinent results from the computations are listed in Table 2. Reference [7] supplied vital information (chemical composition, longitudinal and transverse elastic wave velocities) for the explosives. Reference [6] supplied this information for the PMMA. Appendix A contains the computations for $m_{\rm av}$ and $d_{\rm lav}$ for the explosives and PMMA.

Table 3 lists the computed U_{8f} and P_{8f} results along with pertinent experimental information. Much of the experimental information came from explosive shock pressure sensitivity tests such as the:

- 1. Large scale Gap Tests, LSGT [9]
- 2. Low Amplitude Shock Initiation Tests, LAST [10]
- 3. Modified Gap Test, [8], [13]
- 4. Small Scale Gap Tests, SSGT, [19]

Some very important experimental data came from [11] and [12]. Reference [11] documents a detailed investigation of burning and buildup to detonation in pressed TNT. Shock pressures were generated by impacting the explosives with aluminum plates. The results were also employed in [12] for an analysis of the critical energy concept. In addition, [12] also contains shock velocity information acquired via an explosive wedge technique. This yielded a significant data point which compared well with $U_{\rm af}$ for TNT.

References [14] and [15] document thermocouple temperature measurements in shocked materials. PBX-9404 [14], and PMMA [15], were instrumented with thermocouples and shock loaded at various levels via impact. Above a threshold pressure, the theromocouple maximum output increases rapidly with small increases in shock pressure for both of these materials. These threshold pressure points are listed in Table 3 along with the computed value for Psf. The magnitude comparison is quite good for the PBX-9404, and almost one-to-one for the PMMA.

To facilitate an overall quick visual comparison, Figure 1 illustrates both the computed P_{sf} and the experimental large reaction shock pressure data referred to above and listed in Table 3. In general, P_{sf} is either bracketed by the experimental results or compares rather well with a single experimental point.

It is well known that porosity affects the sensitivity of an explosive to shock induced detonation. In general, less shock pressure is required as the explosive density is decreased or the porosity increases. For examples, see [9], (Figure 4), and [11], [12], and [19]. This observed detonation sensitivity phenomens is believed to be caused by the decrease in V_f , U_{gf} , and P_{gf} as the density decreases. (Section III).

To compute V_f , and hence U_{sf} and P_{sf} , V_l and C_s must be known as a function of ρ_0 . V_l is easy to compute via Eq. (10). C_s is a function of C_l and C_t and these wave velocities will vary with ρ_0 . Sources for C_l and C_t as a function of density for the materials considered herein were unknown to the authors.

Thus, strickly speaking, precise or consistent values of C_8 , V_f , U_{8f} , and P_{8f} as a function of material density could not be computed. However, for Tetryl, a consistent computation was made for one density (ρ_0 = 1.68 Grams/cc) and an approximate computation was made for another density (ρ_0 = 1.50 Grams/cc) (Table 2). V_1 was computed correctly, but C_8 was the same for both densities since C_1 and C_t for ρ_0 = 1.68 Grams/cc was utilized in each case. This makes V_f , U_{8f} , and P_{8f} slightly high for the more porous Tetryl (ρ_0 = 1.50 Gram/cc). P_{8f} for both of these densities is plotted in Figure 2 where they are compared with both LSGT [9] and SSGT [19] results. The comparison is quite good, even though P_{8f} for ρ_0 = 1.5 Grams/cc is somewhat less than shown.

Figure 3 compares the single P_{8f} point computed for TNT (ρ_0 = 1.635 Grams/cc) with available reactive pressure test results acquired for various densities. P_{8f} is less than the comparable equal density SSGT and LSGT results. However, P_{8f} agrees rather well with the reactive (P_R) and detonation threshold (P_D) pressure results reported in [11] which was acquired via aluminum projectile impact testing.

v. CONCLUSIONS

Although this is certainly not an exhaustive investigation, enough information has been presented to indicate that the threshold shock pressures required to initiate reactions leading to detonations in explosives may be related to a critical particle velocity, V_f, sufficient to cause crystal lattice fracture, breakup, and disintegration. Theoretical and experimental results have compared rather well for six high explosives.

The trend of the experimentally observed minimum shock pressure to initiate detonation in explosives as a function of density is consistent with the variation of the crystal lattice fracture shock pressure, $P_{\rm sf}$, with material density. It is shown analytically that $P_{\rm sf}$ decreases as density (ρ_0) decreases, and it is known via experiments that the shock magnitude to cause detonation decreases as the explosive becomes more porous [9] and [19]. $P_{\rm sf}$ computations compare reasonably well with experimental results.

In addition, it has been shown for two materials (PBX-9404 and PMMA) that the shock level at which a greatly enhanced thermocouple output was observed coincides rather well with the computed lattice fracture shock pressure, $P_{\rm Bf}$. In fact for FBX-9404, $P_{\rm Bf}$, $P_{\rm D}$ (detonation threshold), and $P_{\rm R}$ (thermocouple reaction threshold), are all relatively close together. Thus, it is strongly suspected that lattice disintegration and self-sustained phonon fission cause the noticeable increase in temperature and this creates chemical reactions which quickly escaluate to descention. Consequently, it is suggested that other explosives, particularly pressed TNT and Tetryl, be instrumented with thermocouples and tested in the same manner as delineated in [14] and [15].

It is very plausible from a physical viewpoint that crystal lattice disintegration would cause an observable reaction in shocked solids. The rather limited results of this investigation indicate that this phenomena may be responsible for shock induced detonation of solid explosives, and the rather large thermoelectric response of shocked solid materials. Certain observed phase changes in shock loaded materials may be caused by crystal lattice disintegration.

VI. RECOMMENDATIONS

Some recommendations for additional work have already been made, either explicitly, or implicity in the previous sections. For easy reference, these are restated here and some additional recommendations are made.

- A. In addition to PMMA (Plexiglas II, UVA), [15] also contained thermocouple response information for a shocked epoxy, EPON 828. A threshold pressure for enhanced thermocouple output was observed for this material. For comparison, V_f , U_{sf} , and P_{sf} should be computed for EPON 828. This will be done as soon as possible.
- B. In a manner similar to that described in [14] and [15], Comp-B3, Comp-B, pressed TNT, Tetryl, and H-6 should be instrumented with thermocouples and shock loaded at various levels. If the present postulations are valid, these explosives would exhibit an increase in thermocouple response near the $P_{\rm sf}$ pressure level.
- C. Tests have been conducted on pure metals (iron, copper, and aluminum) which were instrumented with thermocouples and shock loaded to rather high pressures via impact [16] and [17]. Similar tests should be systematically conducted at lower shock pressures (30 to 150 kilobars) to ascertain if they exhibit a thermocouple output pressure threshold response point such as observed for PMMA and PBX-9404 near the computed $P_{\rm gf}$ magnitude. $V_{\rm f}$ values for iron, copper and aluminum are given in [2]. Shock and particle velocity information (Co and S) for these metals are given in [3]. Thus, $P_{\rm sf}$, for iron, copper and aluminum can be computed and compared with any appropriate experimental results. This would provide a severe test for the crystal lattice fracture shock pressure, $P_{\rm sf}$, criteria.
- D. Information on the variation of the longitudinal (C_1) and transverse (C_t) elastic wave velocities as a function of density for certain explosives should be acquired, via experimentation if necessary. Information on the variation of U_s , V_s , and U_p as a function of density is also required. Then exact values of V_s , U_{sf} , and P_{sf} as a function of density could be computed and compared with experimental data such as shown in Figures 2 and 3.
- E. The computation of V_1 via Eq. (3), could possibly be refined to take into account atoms and combinations of atoms, and their associated minimum crystal lattice slip distance, which might warrant special attention. This, of course, applies to compounds and mixtures. In the present investigation, average values were computed for the mass of an atom and the distance between them. See Appendix A for these calculations. More sophisticated computations of \mathbf{m}_{av} and \mathbf{d}_1 , should be attempted, for example, to delineate differences in beterogeneous and homogeneous materials.

- F. Permanent lattice distortion or plastic flow occurs for particle velocities between V_1 (Eq. (3)) and V_f (Eq. (1)). Consequently, reactions in explosives (ignition, burning, and even detonation) can occur in this regime. This is a prime topic for further investigation.
- G. The present analysis has not addressed any transient or time dependent phenomena such as the critical energy criteria [18]. However, an investigation, based on concepts presented in [2], should be done to ascertain if the observed time dependence is related to the particle wave motion in a lattice structure.
- H. Reference [21], with its comprehensive review and reference list, is a prime source of topics which should be investigated with respect to shocked crystal lattice disintegration influences. For instance, the authors believe that certain solid-stated shock induced phase changes [22], and shock induced increased chemical reactivity [23], may be caused by the crystal lattice fragmentation phenomena. Lattice breakup and its accompaning self-sustained phonon fission and increased heating are plausible physical conditions for phase changes, increased chemical reactivity, and different electronic characteristics to occur.

TABLE 1. Shocked Material Information.

MATERIAL	<u>00</u>	Co	<u>s</u>	SOURCE
	Grams cm ³	<u>cm</u> µ-sec		-
Comp-B3	1.700	0.303	1.73	Ref. [4]
Comp-B	1.700	0.295	1.67*	Ref. [4]
TNT (Pressed)	1.635	0.208	2.35	Ref. [5]
PBX9404	1.842	0.245	2.48	Ref. [5]
H-6	1.750	0.283	1.70	Ref. [7]
Plexiglas II, UVA (PMMA)	1.180	0.268	1.61	Ref. [6]
Tetryl	1.70	0.2476	1.416	Ref. [20]
Tetryl**	1.50	0.020	4.50	Ref. [20]

^{*}S was modified from 1.58 to 1.67.

^{**} For this density, U_g versus U_p for Tetryl is nonlinear, however, for shock velocities less than 0.19 cm/ μ -sec the above linearization matches the experimental data.

TABLE 2. Numerical Results for Vf. Usf and Psf.

Material	ه ت	d1	V ₁	C1	C.	s,	ΛĘ	Jsa	Psf
	AppA	AprA	Eq. 3			Eq. 4	Eq. 1	Eq. 5	Eq. 6
	(38AMS) #10-23	8_01 10−8	CK II-8ec	CH		C	<u> </u>	CM LI-Sec	KBARS
00MP-83	1.7709	2.1839	0.008571	0.3120	0.1710	0.1612	0.04170	0.3751	26.59
			ro-1.70			1.0=1.726			
COMP-B	1.7494	2.1751	0.008228	0.3120	0.1710	0.1612	0.04077	0.3631	25.16
			ro=1.70			1,0=1.726			
TAT	1.7960	2.2229	0.008299	0.2580	0.1350	0.1310	0.03739	0.2959	18.09
(PRESSEU)			°0=1-635			10=1.635			
PBX-9404	1.757.1	2.1235	0.008879	0.2900	0.1570	0.1491	60170.0	0.3469	26.16
			Co-1.835			('o"1-84			
9-	1.8849	2.2085	0.007959	0.2460	0.1550	0.1345	0.03903	0.3494	34.87
and one			co=1.75			52.1=0.1			
PLEXICLAS	1.2983	.1099	0.01417	0.2711	0.1373	0.1361	6.05157	0.3510	21.36
I, UVA			Co=1.18			81.1=0			
TETR'TI.	1.9072	2.2475	0.007729	0.2270	0.1240	0.1165	0.03411	0.2959	17.00
99-1-03			89•1 -0 ∪			co = 1.68		po=1.68	
TETR YL.	1.9072	2.3340	0.007443	0.2270	0.1240	0.1165	0.03543	0.1794	9.53
ره-۱۰50			05-1-00			1.0=1.68		10=1.50	

* V_{ξ} , $V_{\xi,\xi}$, and P_{Sf} for this porous Tetryl are slightly high since longtudinal (C1) and Transverse (C₁) wave velocity data for Tetryl with v_0 = 1.68 Gram/cm³ were employed to compute C_S and V_{ξ} .

TABLE 3. Theoretical and Experimental Reactive Shock Information Tabulation.

					
Material	l ¹¹ sf	Psf	Exper.	Exper.	Remarks WRT
			Data	Source	Exper. Data
	TABLE 2	TABLE 2	,		
_	<u>cm</u>	KBar	cm/µ-sec	_	
	µ-sec		OT VPom	ļ	
İ	ł		KBar		
Comp-B3	0.3751	26.59	$P_{\rm D} = 22.0$	Ref. 9	Critical detonation
ρο =1.71			-0 -0	(TABLE 11)	initiating pressure
G/cc				, , , , , , , , , , , , , , , , , , , ,	from LSGT* ρ_0 =
	,			j	1.72 G/cc
		·	$P_{R} = 33.0$	Ref. 10	Large reaction
	!			(Fig. 7)	threshold in LASI
}	}				tests**
					ρ _o = 1.702 G/cc
Compa	0.3631	25.16	P 2/ 1	Ref. 9	Critical detonation
Comp-B	0.3031	23.10	$P_{D} = 24.1$	(TABLE 11)	initiating pressure
G/cc				(TABLE II)	from LSGT. Po =
5,55					1.70 G/cc
TNT	0.2959	18.09	$P_{R} = 14.0$	Ref. 11	Coarse Grain
(Pressed)	Í		*	(Fig. 4)	Po = 1.55 G/cc
$\rho_0 = 1.635$					
G/cc			P _R = 15.0	Ref. 11	Fine Grain
i	ŀ		$P_D = 16.1$	(Fig. 4)	ρ _O = 1.55 G/cc
			- 		
	l		U _s = 0.31	Ref. 12	Assymtotic shock
1				(Fig. 10)	velocity for both
					coarse and fine grains. Po =
1	1				1.55 G/cc
1		•	$P_{g} = 24.0$	Ref. 9	Pg from LSGT.
İ			•	(App. C)	$\rho_0^{\circ} = 1.60 \text{ G/cc}$
					(97% TMD)
	1		$P_g = 26.0$	Ref. 9	Pg from LSGT
1				(App. C)	ρ ₀ = 1.640 G/cc
1	ļ	} .	D = 30 0	D-6 13444	(99% TMD)
			P _{GR} = 20.0	1	Reaction, Mod. Gap
1	İ			(Fig. 5) (TABLE 2)	Test, $\rho_0 = 1.60 \text{ G/cc}$
			P _{GD} = 25.0	Ref. 13	Detonation, Mod. Gap
1		}	to	(Fig. 5)	Tests, $\rho_0 = 1.60$
1			30.0	(TABLE 2)	G/cc
PBX-9404	0.3469	26.16	$P_{R} = 30.0$	Ref. 14	Large Reaction thres-
$\rho_0 = 1.835$					hold for thermocouple
G/cc					response po = 1.84
1			D 16 0	<u> </u>	G/cc
			$P_B = 16.0$	Ref. 8	Burning, po =
			$P_{\rm D} = 34.0$	(TABLE 2) Ref. 8	1.83 G/cc Detonation,
	1		· u = 54.0	(TABLE 2)	$\rho_0 = 1.83 \text{ G/cc}$
					ρο 1.05 0/ εξ
	l				<u> </u>

TABLE 3. Theoretical and Experimental Reactive Shock Information
Tabulation (Continued)

	Tabulat	ion . (Conti	ineq)		
Material	Usf	Psí	Exper.	Exper.	Remarks WRT
		• • •	Data	Source	Exper. Data
			cm/µ-sec		[
-	cm	KBar	or	<u>-</u>	
ļ.	u-sec	1	KBar		
į į	y sec		, Kbar	1	
			j	ļ]
 	0.3494	22 07	D = 21 0	D-6 10	D 6 100m
H-6		23.87	Pg = 21.0	Ref. 10	Pg from LSGT
ρ ₀ =1.75	(TABLE 2)	(TABLE 2)		(Fig. 9)	ρ ₀ = 1.77 G/cc
G/cc		İ	ł	}	ł .
			P _R 40.0	Ref. 10	Large reaction
		i		(Fig. 9)	threshold in
1			<u> </u>	1	LASI tests
					$\rho_{0} = 1.77 \text{ G/cc}$
1		·	1	İ	
1			$P_{\chi} = 20.0$	Ref. 9	Pg from LSGT
			6	(App. C)	$\rho_0 = 1.76 \text{ G/cc}$
1				(,)	PRESSED H-6
			Ì		TRESSED II O
			P _g = 30.0	Ref. 9	D from ICCT
1			1 8 2 30.0	*	Pg from LSGT
			}	(App. C)	$\rho_0 = 1.75 \text{ G/cc}$
-	2510	2. 2.		·	Cast H-6
Plexiglas	0.3510	21.36	$P_{R} = 20.0$	Ref. 15	Large Reaction
II, UVA	(TABLE 2)	(TABLE 2)	1	(Fig. 5)	Threshhold for
(PMMA)					thermocouple
			İ		output.
$\rho_0 = 1.18$				1	ρ ₀ = 1.18 G/cc
G/cc				[_	=
Tetryl	0.2959	17.00	$P_g = 15.5$	Ref. 9	LSGT, Estimated
$\rho_0 = 1.68$	(TABLE 2)	(TABLE 2)	°	(Fig. 4)	ρ ₀ = 1.68 G/cc
G/cc	,	,		, ,	
			$P_{50} = 17.5$	Ref. 19	SSGT, *** Exp.
}			}		Data Data
				(P. ClAl)	Po = 1.687 G/cc
1			1	(i · CIRI)	po = 1.00/ 6/66
Tetryl	0.1794	9.53	$P_{o} = 10.0$	Ref. 9	P from ICCT
	(TABLE 2)		Pg = 10.0	1	Pg from LSGT
$\rho_0 = 1.50$	(INDLE 2)	(TABLE 2)	!	(Fig. 4	$\rho_0 = 1.491 \text{ G/cc}$
G/cc				and	
}]	App. C)	ļ
L			<u> </u>	L	

^{*} LSGT - Large Scale Gap Tests (Ref. 9).

^{**} LASI - Low Amplitude Shock Initiation Tests (Ref. 10).

^{***} Reference 13 states that P_{GR} (Reaction Pressure) is sufficient to cause detonation, if the specimen is large enough.

^{****} SSGT - Small Scale Gap Tests (Ref. 19).

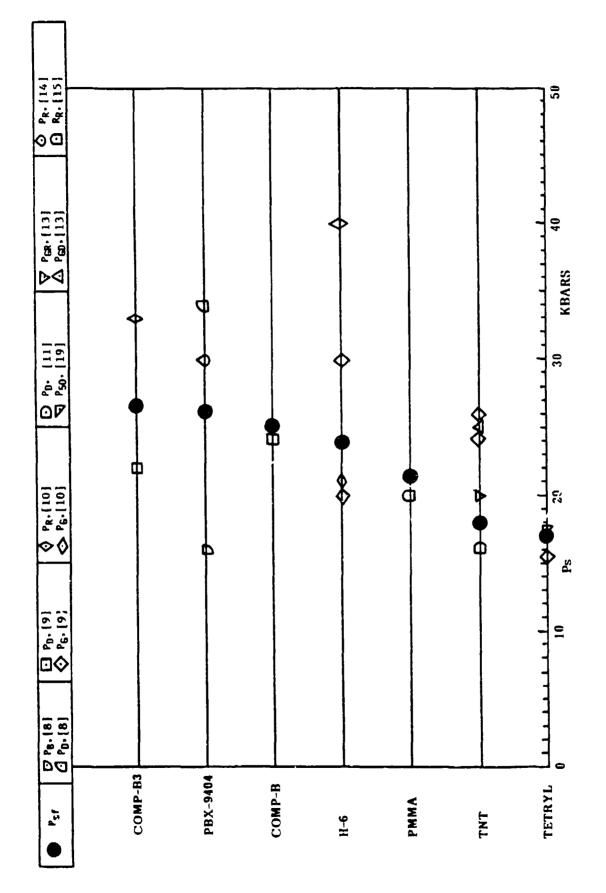


Figure 1. Theoretical and experimental reactive shock pressures.

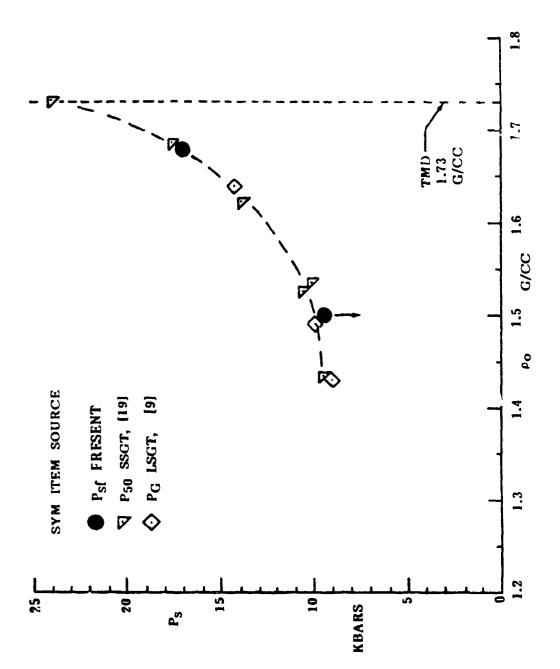


Figure 2. Psf comparison with test results for tetryl.

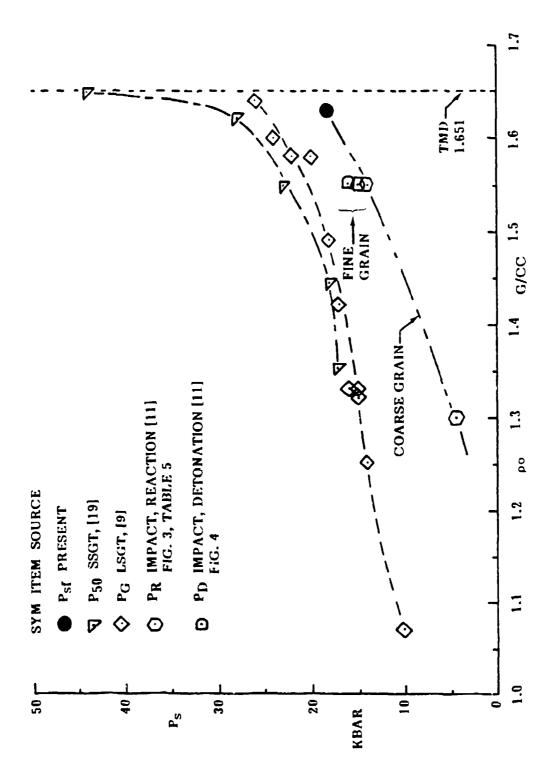


Figure 3. Psf comparison with test results for pressed INT.

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APPENDIX

COMPUTATION OF \mathfrak{m}_{av} AND d_{1av} FOR CHEMICAL COMPOUNDS AND MIXTURES OF COMPOUNDS

The solid materials considered in this study were either chemical compounds (TNT, Tetryl, and PMMA) or mixtures of chemical compounds and pure elements. For these compounds and/or mixtures, the weighted average mass, $m_{\rm av}$, of a single atom in the material was desired.

First, it was necessary to compute the mass of a single atom for each of the elements contained in the solid. Each solid was composed of one or more, but not all, of the following elements:

Carbon, C; Hydrogen, H; Nitrogen, N;

Oxygen, O; Aluminum, Al; Calcium, Ca;

Chlorine, Cl; Phosphorous, P; Flourine, F.

The mass of a single atom of these elements is:

$$m = \frac{MW}{N_{aV}} = \frac{Grams/Gram-Mole}{Atoms/Gram-Mole}$$

Where:

=
$$6.02217 \times 10^{23}$$
 Atoms Gram-Mole

Table A-1 lists MW and m for each of the elements in the above list.

To compute the average weight (m_{av}) of an atom in the material, the chemical formula or proportional chemical composition must be known. Of course, the weight (m) of each elemental atom must also be known, since m_{av} is just a weighted average of the elemental atoms in the material.

When m_{av} is computed, then the average space between atoms (d_{1av}) is given by Eq. (9) in the main text.

$$d_{l_{av}} = \left(\frac{m_{av}}{\rho_o}\right)^{1/3} cm \tag{9}$$

Computations of m_{av} and d_{lav} for the materials considered in this analysis are shown in the following text. Chemical composition information for the explosives was obtained from [7]. Similar information for the inert material (PMMA) was found in [6]. Values of N_{av} and MW are from various chemistry textbooks and handbooks.

TABLE A-1. Mass Of A Single Atom For Selected Elements.

Element	MW	$N_{\mathbf{a}\mathbf{v}}$	m
-	Grams Gram-Mole	Atoms Gram-Mole	Grams Atom
Carbon, C	12.011	6.02252(10 ²³)	1.9943(10 ⁻²³)
Hydrogen, H	1.008		0.1674(10 ⁻²³)
Nitrogen, N	14.008		2.3259(10 ⁻²³)
Oxygen, O	16.00		2.6567(10-23)
Aluminum, Al	26.98		4.4800(10-23)
Calcium, Ca	40.08		$6.6554(10^{-23})$
Chlorine, Cl	35.45		5.8874(10 ⁻²³)
Phosphorous, P	30.97		5.1432(10 ⁻²³)
Flourine, F	18.9984		3.1546(10 ⁻²³)

Comp - B3:
$$\rho_0 = 1.70 \text{ Grams/cm}^3$$

Chemical Composition:
$$C_{2.05}$$
 $H_{2.51}$ $N_{2.15}$ $O_{2.67}$

$$C_{2.05}$$
, 2.05 * 1.9943 (10⁻²³) = 4.0884 (10⁻²³) Grams

$$H_{2.51}$$
, $2.51 * 0.1674 (10^{-23}) = 0.4201 (10^{-23})$ Grams

$$N_{2.15}$$
, 2.15 * 2.3259 (10⁻²³) = 5.0008 (10⁻²³) Grams

$$^{\circ}2.67$$
, $2.67 * 2.6567 (10^{-23}) = 7.0943 (10^{-23})$ Grams

$$m_{av} = \frac{16.6027(10^{-23})}{9.38}$$

= 1.7700
$$(10^{-23})$$
 Grams Atom

$$d_{1av}^3 = \frac{m_{av}}{\rho_0} = \frac{17.700}{1.70} (10^{-24})$$

$$= 10.4118 (10^{-24}) \text{ cm}^3$$

$$d_{1av} = 2.1839 (10^{-8}) \text{ cm}$$

Comp - B:
$$\rho_0 = 1.70 \text{ Grams/cm}^3$$

Chemical Composition:
$$C_{2.03}$$
 $H_{2.64}$ $N_{2.18}$ $O_{2.67}$

$$c_{2.03}$$
, 2.03 * 1.9943 (10⁻²³) = 4.0484 (10⁻²³) Grams

$$H_{2.64}$$
, 2.64 * 0.1674 (10⁻²³) = 0.4419 (10⁻²³) Grams

$$N_{2.18}$$
, 2.18 * 2.3259 (10⁻²³) = 5.0705 (10⁻²³) Grams

$$G_{2.67}$$
, 2.67 * 2.6567 (10⁻²³) = 7.0934 (10⁻²³) Grams

9.52 Atoms
$$16.6542 (10^{-23})$$
 Grams

$$m_{av} = \frac{16.6542 (10^{-23})}{9.52}$$

=
$$1.7494 (10^{-23})$$
 Grams Atoms

$$d_{1av}^3 = \frac{m_{av}}{\rho_0} = \frac{17.494}{1.70} \frac{(10^{-24})}{1.70}$$

$$= 10.2906 (10^{-24}) \text{ cm}^3$$

$$d_{law} = 2.1751 (10^{-8}) cm$$

TNT: $\rho_0 = 1.635 \text{ Grams/cm}^3$

Chemical Composition: C7 H₅ N₃ O₆

$$C_7$$
, 7 * 1.9943 (10⁻²³) = 13.9601 (10⁻²³) Grams

$$H_5$$
, 5 * 0.1674 (10⁻²³) = 0.8370 (10⁻²³) Grams

$$N_3$$
, 3 * 2.3259 (10⁻²³) = 6.9777 (10⁻²³) Grams

$$0_6$$
, 6 * 2.6567 (10⁻²³) = 15.9402 (10⁻²³) Grams

$$\frac{1}{21}$$
 Atoms $\frac{1}{37.7150 (10^{-23})}$ Grams

$$m_{av} = \frac{37.7150 (10^{-23})}{21.0}$$

$$d_{1av}^3 = \frac{m_{AV}}{\rho o} = \frac{17.9595 (10^{-24})}{1.635}$$

$$= 10.9844 \text{ cm}^3$$

$$d_{1av} = 2.2229 (10^{-8}) \text{ cm}$$

PBX - 9404: $\rho_0 = 1.835 \text{ Grams/cm}^3$

Chemical Composition: $C_{1.40} H_{2.75} N_{2.57} O_{2.69} Cl_{0.03} P_{0.01}$

$$C_{1.40}$$
 1.40 * 1.9943 (10⁻²³) = 2.79202 (10⁻²³) Grams

$$H_{2.75}$$
 2.75 * 0.1674 (10⁻²³) = 0.46035 (10⁻²³) Grams

$$N_{2.57}$$
 2.57 * 2.3259 (10⁻²³) = 5.97756 (10⁻²³) Grams

$$02.69$$
 2.69 * 2.6567 (10⁻²³) = 7.14652 (10⁻²³) Grams

$$c_{10.03}$$
 0.03 * 5.8874 (10⁻²³) = 0.17662 (10⁻²³) Grams

$$P_{0.01}$$
 0.01 * 5.1432 (10⁻²³) = 0.05143 (10⁻²³) Grams

$$m_{av} = \frac{16.6045 (10^{-23})}{9.45}$$

$$\sim 1.7571 (10^{-23}) \frac{Grams}{Atom}$$

$$d_{1av} = \frac{m_{av}}{\rho_{0}} = \frac{17.571 (10^{-24})}{1.835}$$

$$= 9.5754 (10^{-24}) \text{ cm}^3$$

$$d_{1_{av}} = 2.1235 (10^{-8})$$
 cm

H-6: $\rho_0 = 1.75 \text{ Grams/cm}^3$

Chemical Composition: $C_{1.89}$ $H_{2.59}$ $N_{1.61}$ $O_{2.01}$ $Al_{0.74}$ $Ca_{0.005}$ $Cl_{0.009}$

$$C_{1.89}$$
 1.89 * 1.9943 (10⁻²³) = 3.7692 (10⁻²³) Grams

$$H_{2.59}$$
 2.59 * 0.1674 (10⁻²³) = 0.4336 (10⁻²³) Crams

$$N_{1.61}$$
 1.61 * 2.3259 (10⁻²³) = 3.7447 (10⁻²³) Grams

$$0_{2.01}$$
 2.01 * 2.6567 (10⁻²³) = 5.3400 (10⁻²³) Grams

$$A1_{0.74}$$
 0.74 * 4.4800 (10⁻²³) = 3.3152 (10⁻²³) Grams

$$Ca_{0.005} = 0.005 * 6.6554 (10^{-23}) = 0.0328 (10^{-23})$$
 Grams

C10.009 0.009 * 5.8874 (10⁻²³) • 0.0530 (10⁻²³) Grams
$$\frac{16.6685 (10^{-23})}{8.854} \text{ Atoms}$$

$$m_{av} = \frac{16.6885 (10^{-23})}{8.854}$$

$$= 1.8849 (10^{-23}) \frac{Grams}{Atom}$$

$$d_{1_{av}}^3 = \frac{m_{av}}{\rho_0} = \frac{18.849 (10^{-24})}{1.75}$$

$$= 16.7712 (10^{-24}) \text{ cm}^3$$

$$d_{l_{av}} = 2.2085 (10^{-8}) \text{ cm}$$

TETRYL: $\rho_0 = 1.68$ Grams/cm³

Chemical Composition: C7 H5 N5 O8

$$C_7$$
, 7 * 1.9943 (10⁻²³) = 13.9601 (10⁻²³) Grams

$$H_5$$
, 5 * 0.1674 (10⁻²³) = 9.8370 (10⁻²³) Grams

$$N_5$$
, 5 * 2.3259 (10⁻²³) = 11.6295 (10⁻²³) Grams

$$0_8$$
, 8 * 2.6567 (10⁻²³) = 21.2536 (10⁻²³) Grams

$$m_{av} = \frac{47.6802 (10^{-23})}{25}$$

= 1.9072 (
$$10^{-23}$$
) Grams Atom

$$d_{1_{av}}^3 = \frac{m_{av}}{\rho_0} = \frac{19.072 \quad (10^{-24})}{1.68}$$

$$= 11.3524 (10^{-24}) \text{ cm}^3$$

$$d_{l_{RV}} = 2.2475 (10^{-8}) \text{ cm}$$

POLYMETHYL - METHACRYLATE (PMMA) (PLEXIGLAS TYPE II, UVA)

$$\rho_0 = 1.18 \frac{Gram}{cm^3}$$

Chemical Composition: $(C_5 \text{ Hg } O_2)_N$

$$C_5$$
, 5 * 1.9943 (10⁻²³) = 9.9715 (10⁻²³) Grams

H₈, 8 * 0.1674
$$(10^{-23})$$
 = 1.3392 (10^{-23}) Grams

$$O_2$$
, 2 * 2.6567 (10⁻²³) = 5.3134 (10⁻²³) Grams

$$m_{av} = \frac{16.6241 (10^{-23})}{15.0}$$

$$d_{1av}^3 = \frac{m_{av}}{\rho_0} = \frac{11.083 (10^{-24})}{1.18}$$

$$= 9.3924 (10^{-24}) \text{ cm}^3$$

$$d_{1_{8V}} = 2.1099 (10^{-8}) \text{ cm}$$

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